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NUMERICAL APPROXIMATION FOR THE FRACTIONAL DIFFUSION EQUATION VIA SPLINES

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ABSTRACT: A one dimensional fractional diffusion model is considered, where the usual second-order derivative gives place to a fractional derivative of order α, with $1 < \alpha \leq 2$. We consider the Caputo derivative as the space derivative, which is a form of representing the fractional derivative by an integral operator. The numerical solution is derived using Crank-Nicolson method in time combined with a spline approximation for the Caputo derivative in space. Consistency and convergence of the method is examined and numerical results are presented.

1. Introduction

To derive numerical solutions for differential equations of integer order has for a long time been a topic in computational sciences. Recently, a large number of applied problems have been formulated on fractional differential equations and there is still a lack of highly accurate numerical methods for this type of equations. In this paper we are concerned with a fractional diffusion model with a spatial derivative of fractional order α, $1 < \alpha \leq 2$. When this fractional derivative replaces the second order derivative in a diffusion model it leads to enhanced diffusion, also called superdiffusion [8]. Recent work on numerical solutions for this particular problem can be found in [11, 14].

Fractional diffusion equations account for the typical anomalous features which are observed in many problems. A numerical approach to different types of fractional diffusion models have been increasingly appearing in literature. A fractional diffusion equation describing subdiffusion is studied for instance in [1, 15, 16]. In [3] additionally to the fractional order derivative a nonlocal quadratic nonlinearity is considered. Several transport equations include a fractional order diffusion derivative [4, 7, 13, 18]. Other models consider also for advection a fractional derivative of order $0 < \beta \leq 1$ [6, 12].

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The numerical methods developed until now for fractional partial differential equations which involves a derivative of order α, $1 < \alpha \leq 2$ are mainly of order one. A numerical method of order two can be found in [14], where a first order approximation of the fractional derivative is derived and a Richardson's extrapolation is applied to achieve second-order accuracy.

In this work we present a second order approximation for the fractional derivative of order α, $1 < \alpha < 2$. Additionally by doing an implicit discretisation in time we present a numerical method with a full discretization of second order.

Consider the one-dimensional fractional diffusion equation

$$\frac{\partial u}{\partial t}(x,t) = d(x)\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) + p(x,t) \tag{1}$$

on a finite domain $a < x < b$, where $1 < \alpha < 2$ and $d(x) > 0$. We consider the initial condition

$$u(x,0) = f(x), \;\; a < x < b \tag{2}$$

and Dirichlet boundary conditions

$$u(a,t) = g_a(t) \quad \text{and} \quad u(b,t) = g_b(t). \tag{3}$$

The usual way of representing the fractional derivatives is by the Riemann-Liouville formula. The Riemann-Liouville fractional derivative of order α, for $x \in [a,b]$, $-\infty \leq a < b \leq \infty$, is defined by

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_a^x u(\xi,t)(x-\xi)^{n-\alpha-1}d\xi, \quad (n-1 < \alpha < n) \tag{4}$$

where $\Gamma(\cdot)$ is the Gamma function and $n = [\alpha]+1$, with $[\alpha]$ denoting the integer part of α. Another way to represent the fractional derivatives is by the Grünwald-Letnikov formula, that is,

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \lim_{\Delta x \to 0}\frac{1}{\Delta x^\alpha}\sum_{k=0}^{\left[\frac{x-a}{\Delta x}\right]}(-1)^k \begin{pmatrix} \alpha \\ k \end{pmatrix} u(x-k\Delta x,t). \quad (\alpha > 0) \tag{5}$$

The discrete approximations of the Grünwald-Letnikov fractional derivative present some limitations. First, numerical approximations based in this formula very frequently originates unstable numerical methods and henceforth many times a shifted Grünwald-Letnikov formula is used. Another disadvantage is that the order of accuracy of such approaches is never higher than one.

A different representation of the fractional derivative was proposed by Caputo,

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \frac{1}{\Gamma(n-\alpha)} \int_a^x \frac{\partial^n u}{\partial \xi^n}(\xi,t)(x-\xi)^{n-\alpha-1} d\xi, \quad (n-1<\alpha<n) \quad (6)$$

where $n = [\alpha]+1$. The Caputo representation has some advantages over the Riemann-Liouville representation. The most well known is related with the fact that very frequently the Laplace transform method is used for solving fractional differential equations. The Laplace transform of the Riemann-Liouville derivative leads to boundary conditions containing the limit values of the Riemann-Liouville fractional derivatives at the lower terminal $x = a$. In spite of the fact that mathematically such problems can be solved, there is no physical interpretation for such type of conditions. On the other hand the Laplace transform of the Caputo derivative imposes boundary conditions involving integer-order derivatives at the lower point $x = a$ which usually are acceptable physical conditions. Another advantage is that the Caputo derivative of a constant is zero, whereas for the Riemann-Liouville is not. Properties about the fractional derivatives can be found for instance in [5, 9, 10]. We consider the Caputo representation to derive a numerical approximation for the fractional derivative.

The plan of the paper is as follows. In section 2 we derive a linear spline approximation for the Caputo derivative. The full discretisation of the fractional diffusion equation is given in section 3, where we apply Crank-Nicolson in time. In section 4 we prove the convergence of the numerical method by showing it is consistent and C-stable and in the last section we present numerical results which confirm the numerical method is second order accurate.

2. The spline approximation of the Caputo derivative

In this section we derive a numerical approximation to the Caputo derivative for $a < x < b$,

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \frac{1}{\Gamma(2-\alpha)} \int_a^x \frac{\partial^2 u}{\partial \xi^2}(\xi,t)(x-\xi)^{1-\alpha} d\xi, \quad 1<\alpha<2. \quad (7)$$

Let us define the mesh points

$$x_j = a + j\Delta x, \ j = 0, 1 \ldots, N$$

where Δx denotes the uniform space step.

For $x_j,\ j = 1, \ldots, N-1$ we need to calculate

$$\frac{1}{\Gamma(2-\alpha)} \int_a^{x_j} \frac{\partial^2 u}{\partial \xi^2}(\xi, t)(x_j - \xi)^{1-\alpha} d\xi, \quad j = 1, \ldots, N-1. \tag{8}$$

We compute these integrals by approximating the second order derivative by a linear spline $s_j(\xi)$, whose nodes and knots are chosen at x_k, $k = 0, 1, 2, \ldots, j$, that is, an approximation to (8) becomes

$$I_j = \frac{1}{\Gamma(2-\alpha)} \int_a^{x_j} s_j(\xi)(x_j - \xi)^{1-\alpha} d\xi. \tag{9}$$

The spline $s_j(\xi)$ interpolates

$$\frac{\partial^2 u}{\partial \xi^2}(x_0, t), \ldots, \frac{\partial^2 u}{\partial \xi^2}(x_j, t)$$

and is of the form

$$s_j(\xi) = \sum_{k=0}^{j} \frac{\partial^2 u}{\partial \xi^2}(x_k, t) s_{j,k}(\xi), \tag{10}$$

with $s_{j,k}(\xi)$, in each interval $[x_{k-1}, x_{k+1}]$, for $1 \leq k \leq j-1$, given by

$$s_{j,k}(\xi) = \begin{cases} \dfrac{\xi - x_{k-1}}{x_k - x_{k-1}}, & x_{k-1} \leq \xi \leq x_k \\[2ex] \dfrac{x_{k+1} - \xi}{x_{k+1} - x_k}, & x_k \leq \xi \leq x_{k+1} \\[2ex] 0 & \text{otherwise.} \end{cases}$$

For $k = 0$ and $k = j$, $s_{j,k}(\xi)$ is of the form

$$s_{j,0}(\xi) = \begin{cases} \dfrac{x_1 - \xi}{x_1 - x_0}, & x_0 \leq \xi \leq x_1 \\[2ex] 0 & \text{otherwise} \end{cases} \qquad s_{j,j}(\xi) = \begin{cases} \dfrac{\xi - x_{j-1}}{x_j - x_{j-1}}, & x_{j-1} \leq \xi \leq x_j \\[2ex] 0 & \text{otherwise.} \end{cases}$$

From (9) and (10), we have

$$I_j = \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{j} \frac{\partial^2 u}{\partial \xi^2}(x_k, t) \int_a^{x_j} (x_j - \xi)^{1-\alpha} s_{j,k}(\xi) d\xi,$$

and after some calculations we obtain

$$I_j = \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{k=0}^{j} \frac{\partial^2 u}{\partial \xi^2}(x_k, t) a_{j,k}, \tag{11}$$

where

$$a_{j,k} = \begin{cases} (j-1)^{3-\alpha} - j^{2-\alpha}(j-3+\alpha), & k=0 \\ (j-k+1)^{3-\alpha} - 2(j-k)^{3-\alpha} + (j-k-1)^{3-\alpha} & 1 \leq k \leq j-1 \\ 1 & k=j. \end{cases} \tag{12}$$

Let us assume there are approximations $\mathbf{U}^n := \{U_j^n\}$ to the values $u(x_j, t_n)$, where $t_n = n\Delta t,\ n \geq 0$ and Δt is the uniform time-step. For the mesh points $x_k, k = 1, \ldots, N-1$ the second order derivative of (11) can be approximated by $\delta^2 U_j^n / \Delta x^2$ where δ^2 is the central second order differential operator

$$\delta^2 U_j^n = U_{j+1}^n - 2U_j^n + U_{j-1}^n.$$

Additionally, we also need to know the value of the second order derivative at the boundary point x_0. If we have a physical boundary condition of the type

$$\frac{\partial^2 u}{\partial x^2}(x_0, t) = b(t) \tag{13}$$

we can consider the given value. Unfortunately this is not a usual physical boundary condition. Therefore at $x = x_0$ the second order derivative can be approximated by $\delta_0 U_0 / \Delta x^2$ where δ_0 is the operator

$$\delta_0 U_j^n = 2U_j^n - 5U_{j+1}^n + 4U_{j+2}^n - U_{j+3}^n. \tag{14}$$

A discrete approximation at a boundary point is usually called a numerical boundary condition.

Finally, the approximation of I_j for $t = t_n$ can be written as

$$I_j \simeq \frac{\Delta x^{-\alpha}}{\Gamma(4-\alpha)} \left\{ a_{j,0} \delta_0 U_0^n + \sum_{k=1}^{j} a_{j,k} \delta^2 U_k^n \right\}.$$

In this section we have considered a linear spline to approximate the integral representation of the Caputo derivative with the purpose of obtaining a second order approximation. Nevertheless a higher order approximation can be achieved by using a quadratic or cubic spline, although we may not be able to have explicit forms similar to (11), (12).

In the next section we describe the full discretisation of the differential equation and write the matricial form of our numerical method.

3. The numerical scheme

We discretize the spatial α-order derivative following the steps of the previous section. The discretization in time consists of the Crank-Nicolson numerical method. We consider the time discretization $0 \le t_n \le T$. Additionally, let $d_j = d(x_j)$ and $p_j^{n+1/2} = p(x_j, t_{n+1/2})$, where $t_{n+1/2} = t_n + (1/2)\Delta t$. For the uniform space step Δx and time step Δt, let

$$\mu_j^\alpha = \frac{d_j \Delta t}{\Delta x^\alpha}.$$

The fractional differential operator is defined as

$$\delta_\alpha U_j^n = \frac{1}{\Gamma(4-\alpha)} \left\{ a_{j,0}\delta_0 U_0^n + \sum_{k=1}^{j} a_{j,k}\delta^2 U_k^n \right\}.$$

We have the following numerical method

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{d_j}{2\Delta x^\alpha}\left(\delta_\alpha U_j^{n+1} + \delta_\alpha U_j^n\right) + p_j^{n+1/2}, \tag{15}$$

that is,

$$\left(1 - \frac{\mu_j^\alpha}{2}\delta_\alpha\right) U_j^{n+1} = \left(1 + \frac{\mu_j^\alpha}{2}\delta_\alpha\right) U_j^n + p_j^{n+1/2}\Delta t. \tag{16}$$

The numerical method can be written in the matricial form

$$(I - \mathbf{Q})\mathbf{U}^{n+1} = (I + \mathbf{Q})\mathbf{U}^n + \mathbf{b}^{n+1} + \mathbf{b}^n + \mathbf{p}^{n+1/2}, \tag{17}$$

where $\mathbf{U}^n = \left[U_1^n \dots U_{N-1}^n\right]^T$, $\mathbf{p}^{n+1/2} = \left[\Delta t p_1^{n+1/2} \dots \Delta t p_{N-1}^{n+1/2}\right]^T$, $\mathbf{b}^n$ contains the boundary values and $\mathbf{Q}$ is related to the fractional operator. The matrix $\mathbf{Q}$ has the following structure

$$\mathbf{Q} = \mathbf{M} + \mathbf{N},$$

where the matrix $\mathbf{M}$ is related to the operator δ^2 and the matrix $\mathbf{N}$ is related to the operator δ_0. The matrices $\mathbf{M} = [M_{j,k}]$ and $\mathbf{N} = [N_{j,k}]$ are of the form:

$$M_{j,k} = \frac{\mu_j^\alpha}{2\Gamma(4-\alpha)} \begin{cases} -2a_{1,1}, & j=1,\ k=1 \\ -2a_{j,1} + a_{j,2}, & 2 \le j \le N-1,\ k=1 \\ a_{j,k-1} - 2a_{j,k} + a_{j,k+1}, & k \le j-1,\ k \ge 2 \\ a_{j,j-1} - 2a_{j,j}, & k = j,\ k \ge 2 \\ a_{j,j}, & k = j+1,\ k \ge 2 \\ 0, & k > j+1,\ k \ge 2 \end{cases}$$

and, for $1 \le j \le N-1$,

$$N_{j,k} = \frac{\mu_j^\alpha}{2\Gamma(4-\alpha)} \begin{cases} -5a_{j,0}, & k=1 \\ 4a_{j,0}, & k=2 \\ -a_{j,0}, & k=3 \\ 0, & k \ge 4. \end{cases}$$

Finally the vector $\mathbf{b}^n$ is given by

$$b_j^n = \frac{\mu_j^\alpha}{2\Gamma(4-\alpha)} \begin{cases} (2a_{j,0} + a_{j,1})U_0^n, & j = 1, \ldots, N-2 \\ (2a_{j,0} + a_{j,1})U_0^n + a_{j,j}U_N^n, & j = N-1. \end{cases}$$

Note that $U_0^n = g_a(t_n)$ and $U_N^n = g_b(t_n)$. Additionally, if we assume the condition (13) is given, then we have $\mathbf{Q} = \mathbf{M}$.

4. Consistency and convergence of the numerical scheme

We first start to study the consistency of the numerical method and lastly we present the convergence results. Let $C^3[a,b]$ be the linear space of real valued functions on $[a,b]$ that have continuous third order derivatives.

Theorem 1. *Let $u^n(x)$ be a function in $C^3[a,b]$ and $1 < \alpha < 2$. Consider the discrete operator δ_α defined by*

$$\delta_\alpha u^n(x_j) = \frac{1}{\Gamma(4-\alpha)} \left(a_{j,0}\delta_0 u^n(x_0) + \sum_{k=1}^{j} a_{j,k}\delta^2 u^n(x_k) \right),$$

where $\delta_0 u^n(x_k) = 2u^n(x_k) - 5u^n(x_{k+1}) + 4u^n(x_{k+2}) - u^n(x_{k+3})$ and $\delta^2 u^n(x_k) = u^n(x_{k+1}) - 2u^n(x_k) + u^n(x_{k-1})$. Then

$$\frac{1}{\Delta x^\alpha}\delta_\alpha u^n(x_j) = \frac{\partial^\alpha u^n}{\partial x^\alpha}(x_j) + \epsilon_1(x_j) + \epsilon_2(x_j)$$

with

$$\max_{a\leq x_j\leq b}|\epsilon_p(x_j)| \leq \frac{(b-a)^{2-\alpha}}{\Gamma(3-\alpha)}\mathcal{O}(\Delta x^2), \quad p=1,2.$$

Proof: Considering the definition of the operator δ_α, we have

$$\frac{1}{\Delta x^\alpha}\delta_\alpha u^n(x_j) = \frac{\Delta x^{-\alpha}}{\Gamma(4-\alpha)}\left(a_{j,0}\delta_0 u^n(x_0) + \sum_{k=1}^{j} a_{j,k}\delta^2 u^n(x_k)\right).$$

Now, using Taylor expansion arguments it is easy to check that

$$\frac{1}{\Delta x^2}\delta_0 u^n(x_0) = \frac{d^2u}{dx^2}(x_0) + \mathcal{O}(\Delta x^2); \quad \frac{1}{\Delta x^2}\delta^2 u^n(x_k) = \frac{d^2u}{dx^2}(x_k) + \mathcal{O}(\Delta x^2).$$

Therefore

$$\begin{aligned}\frac{1}{\Delta x^\alpha}\delta_\alpha u^n(x_j) &= \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)}\sum_{k=0}^{j} a_{j,k}\left(\frac{d^2u^n}{dx^2}(x_k) + \mathcal{O}(\Delta x^2)\right)\\ &= \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)}\sum_{k=0}^{j} a_{j,k}\frac{d^2u^n}{dx^2}(x_k) + \epsilon_1(x_j)\end{aligned}$$

with

$$\epsilon_1(x_j) = \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)}\sum_{k=0}^{j} a_{j,k}\mathcal{O}(\Delta x^2) = \frac{(x_j-a)^{2-\alpha}}{\Gamma(3-\alpha)}\mathcal{O}(\Delta x^2).$$

We can write

$$\begin{aligned}\frac{1}{\Delta x^\alpha}\delta_\alpha u^n(x_j) &= \frac{1}{\Gamma(2-\alpha)}\int_a^{x_j} s_j(\xi)(x_j-\xi)^{1-\alpha}d\xi + \epsilon_1(x_j)\\ &= \frac{1}{\Gamma(2-\alpha)}\int_a^{x_j} \frac{d^2u^n}{dx^2}(\xi)(x_j-\xi)^{1-\alpha}d\xi + \epsilon_2(x_j) + \epsilon_1(x_j),\end{aligned}$$

for

$$\epsilon_2(x_j) = \frac{1}{\Gamma(2-\alpha)}\left|\int_a^{x_j} s_j(\xi)(x_j-\xi)^{1-\alpha}d\xi - \int_a^{x_j}\frac{d^2u^n}{dx^2}(\xi)(x_j-\xi)^{1-\alpha}d\xi\right|$$

and henceforth

$$\epsilon_2(x_j) \leq \frac{1}{\Gamma(2-\alpha)}\max_{a\leq\xi\leq b}\left|\frac{d^2u^n}{dx^2}(\xi) - s_j(\xi)\right|\int_a^{x_j}(x_j-\xi)^{1-\alpha}d\xi.$$

The function $s_j(\xi)$ is a piecewise linear approximation for $\dfrac{d^2u^n}{dx^2}$ and it is known that

$$\max_{a\leq\xi\leq b}\left|\frac{d^2u^n}{dx^2}(\xi)-s_j(\xi)\right|=\mathcal{O}(\Delta x^2)$$

and therefore

$$\epsilon_2(x_j)\leq\frac{(x_j-a)^{2-\alpha}}{\Gamma(3-\alpha)}\mathcal{O}(\Delta x^2).$$

■

The next result shows the numerical scheme (16) is second order accurate.

Proposition 2. *The numerical scheme (16) is of order $\mathcal{O}(\Delta x^2)+\mathcal{O}(\Delta t^2)$.*

Proof: Let $u=u(x,t)$ be a solution to the fractional partial differential equation (1) and note that the truncation error is given by

$$\tau_j^n=\frac{u_j^{n+1}-u_j^n}{\Delta t}-\frac{d_j}{2\Delta x^\alpha}\left(\delta_\alpha u_j^{n+1}+\delta_\alpha u_j^n\right)-p_j^{n+1/2}.$$

Thus, taking in consideration the previous theorem, we have

$$\begin{aligned}\tau_j^n &= \left(\frac{\partial u}{\partial t}\right)_j^{n+1/2}+\mathcal{O}(\Delta t^2)-d_j\left(\frac{\partial^\alpha u}{\partial x^\alpha}\right)_j^{n+1/2}+\mathcal{O}(\Delta x^2)+\mathcal{O}(\Delta t^2)-p_j^{n+1/2}\\ &= \left(\frac{\partial u}{\partial t}\right)_j^{n+1/2}-d_j\left(\frac{\partial^\alpha u}{\partial x^\alpha}\right)_j^{n+1/2}-p_j^{n+1/2}+\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2),\end{aligned}$$

and therefore

$$\tau_j^n=\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2).$$

■

To prove the convergence of the numerical scheme we apply the following theorem ([17], pg. 304).

Theorem 3. *Suppose that the full discretization is consistent and the integration method is C-stable. Then the full discretization is convergent.*

To prove the convergence of the numerical method, since we have already proved the discretization is consistent, we need to prove the integration method is C-stable.

We start to define C-stability. Let U^n and $\tilde{U}^n$ be two solutions of the numerical method (16).

Definition 1.([2]) Let $||\cdot||$ be a norm on $\mathbb{R}^m$. The integration method is called C-stable with respect to this norm if a positive real number $\Delta t_0 = \Delta t_0(\Delta x)$ and a real constant C_0 independent of Δt and Δx exist, such that for $\Delta t \in (0, \Delta t_0]$ and each $\tilde{U}^n, U^n \in \mathbb{R}^m$

$$||\tilde{U}^{n+1} - U^{n+1}|| \leq (1 + C_0 \Delta t)||\tilde{U}^n - U^n||.$$

To prove the numerical method is C-stable we consider the infinity norm $||\cdot||_\infty$. Therefore, firstly we derive bounds for the infinity norm of the matrices $\mathbf{M}$ and $\mathbf{Q}$ that appear in the numerical method (17).

Proposition 4. *Let* $||\mu^\alpha||_\infty = \max\limits_{1\leq j\leq N-1} \mu_j^\alpha$.

(a) Let $3 \leq m_{\max}(\alpha) \leq 4$. *The infinity norm of the matrix* $\mathbf{M}$ *is bounded by*

$$||\mathbf{M}||_\infty \leq \frac{||\mu^\alpha||_\infty}{2\Gamma(4-\alpha)} m_{\max}(\alpha). \tag{18}$$

(b) The infinity norm of the matrix $\mathbf{Q}$ *is bounded by*

$$||\mathbf{Q}||_\infty \leq \frac{||\mu^\alpha||_\infty}{2\Gamma(4-\alpha)} q_{\max}(\alpha), \tag{19}$$

for

$$q_{\max}(\alpha) = \begin{cases} 10(2-\alpha)+3, & 1 < \alpha \leq \alpha^* \\ 3^{3-\alpha} + 5(2^{3-\alpha}) + 4^{2-\alpha}(-9\alpha+3) + 6, & \alpha^* \leq \alpha < 2 \end{cases}$$

where α^* *is the intersection point between the two curves. The value of* α^* *is approximately* 1.9118.

Proof: (a) Let us define $\mathbf{M}^* = [M^*_{j,k}]$, such that

$$M^*_{1,1} = -2a_{1,1}, \quad M^*_{j,1} = -2a_{j,1} + a_{j,2}, \; 2 \leq j \leq N-1$$

and for $1 \leq j \leq N-1$, $k \geq 2$

$$M^*_{j,k} = \begin{cases} a_{j,k-1} - 2a_{j,k} + a_{j,k+1}, & k \leq j-1 \\ a_{j,j-1} - 2a_{j,j}, & k = j \\ a_{j,j}, & k = j+1 \\ 0, & k > j+1. \end{cases}$$

For $\mathbf{M} = [M_{j,k}]$, we have

$$M_{j,k} = \frac{1}{2\Gamma(4-\alpha)} \mu_j^\alpha M_{j,k}^*.$$

and

$$||\mathbf{M}||_\infty \leq \frac{||\mu^\alpha||_\infty}{2\Gamma(4-\alpha)} ||\mathbf{M}^*||_\infty.$$

Since $M_{j,k}^* = 0$, for $k \geq j+1$, then

$$||\mathbf{M}^*||_\infty = \max_{1\leq j\leq N-1} \left[\sum_{k=1}^{N-1} |M_{j,k}^*| \right] = \max_{1\leq j\leq N-1} \left[\sum_{k=1}^{j+1} |M_{j,k}^*| \right] = \max_{1\leq j\leq N-1} M_j^*,$$

with

$$M_j^* = \sum_{k=1}^{j+1} |M_{j,k}^*|.$$

We evaluate separately M_1^*, M_2^*, M_3^*, M_4^* and M_j^* for $j \geq 5$. We obtain

$$M_1^* = 3; \qquad M_2^* = \begin{cases} a_{2,1} + 2a_{2,2}, & 1 < \alpha \leq 4 - \ln_2(5) \\ -3a_{2,1} + 4a_{2,2}, & 4 - \ln_2(5) \leq \alpha < 2. \end{cases}$$

For α_1 and α_2 such that $3^{3-\alpha_1} - 4(2^{3-\alpha_1}) + 6 = 0$ and $2(3^{3-\alpha_2}) - 5(2^{3-\alpha_2}) + 4 = 0$ we have $1 < \alpha_1 < \alpha_2 < 2$ and M_3^* given by

$$M_3^* = \begin{cases} a_{3,1} + 2a_{3,3}, & 1 < \alpha \leq \alpha_1 \\ 3a_{3,1} - 4a_{3,2} + 4a_{3,3}, & \alpha_1 \leq \alpha \leq \alpha_2 \\ -a_{3,1} - 2a_{3,2} + 4a_{3,3}, & \alpha_2 \leq \alpha < 2. \end{cases}$$

Note that $\alpha_1 \simeq 1.5545$ and $\alpha_2 \simeq 1.7606$. We also have

$$M_4^* = \begin{cases} 3a_{4,1} - 4a_{4,2} + 2a_{4,3} + 2a_{4,4}, & 1 < \alpha \leq \alpha_1 \\ 3a_{4,1} - 2a_{4,2} - 2a_{4,3} + 4a_{4,4}, & \alpha_1 \leq \alpha < 2 \end{cases}$$

and for $j \geq 5$

$$M_j^* = \begin{cases} 3a_{j,1} - 2a_{j,2} - 2a_{j,j-2} + 2a_{j,j-1} + 2a_{j,j}, & 1 < \alpha \leq \alpha_1 \\ 3a_{j,1} - 2a_{j,2} - 2a_{j,j-1} + 4a_{j,j}, & \alpha_1 \leq \alpha < 2. \end{cases}$$

After some calculations it is easy to check that for all j and for all $1 < \alpha < 2$,

$$3 \leq M_j^* \leq 4.$$

Therefore $||\mathbf{M}^*||_\infty \leq m_{\max}(\alpha)$ for $3 \leq m_{\max}(\alpha) \leq 4$.

(b) Let $\mathbf{Q}^* = \mathbf{M}^* + \mathbf{N}^*$, where $\mathbf{N}^* = [N^*_{j,k}]$ is given by

$$N^*_{j,k} = \begin{cases} -5a_{j,0}, & k = 1 \\ 4a_{j,0}, & k = 2 \\ -a_{j,0}, & k = 3 \\ 0, & k \geq 4. \end{cases}$$

For $\mathbf{Q} = [q_{j,k}]$ and $\mathbf{Q}^* = [q^*_{j,k}]$, we have

$$q_{j,k} = \frac{1}{2\Gamma(4-\alpha)} \mu_j^\alpha q^*_{j,k}.$$

Therefore

$$||\mathbf{Q}||_\infty \leq \frac{||\mu^\alpha||_\infty}{2\Gamma(4-\alpha)} ||\mathbf{Q}^*||_\infty.$$

Since $q^*_{j,k} = 0$, for $k \geq j+1$, then

$$||\mathbf{Q}^*||_\infty = \max_{1 \leq j \leq N-1} \left[\sum_{k=1}^{N-1} |q^*_{j,k}| \right] = \max_{1 \leq j \leq N-1} \left[\sum_{k=1}^{j+1} |q^*_{j,k}| \right] = \max_{1 \leq j \leq N-1} Q^*_j,$$

where

$$Q^*_j = \sum_{k=1}^{j+1} |q^*_{j,k}| = \sum_{k=1}^{j+1} |M^*_{j,k} + N^*_{j,k}| = \sum_{k=1}^{3} |M^*_{j,k} + N^*_{j,k}| + \sum_{k=4}^{j+1} |M^*_{j,k}|.$$

After some algebraic calculations we obtain

$$Q^*_1 = 10(2-\alpha) + 3; \qquad Q^*_2 = \begin{cases} 8a_{2,0} + 3a_{2,1} - 2a_{2,2}, & 1 < \alpha \leq 3/2 \\ -2a_{2,0} + a_{2,1} + 2a_{2,2}, & 3/2 \leq \alpha \leq 9/5 \\ -10a_{2,0} - 3a_{2,1} + 4a_{2,2}, & 9/5 \leq \alpha < 2 \end{cases}$$

$$Q^*_3 = 10a_{3,0} + 3a_{3,1} - 4a_{3,2} + 4a_{3,3}.$$

For α_3 and α_4 such that $-4(2^{3-\alpha_3}) + 4^{2-\alpha_3}(1-\alpha_3) + 6 = 0$ and $-4(3^{3-\alpha_4}) + 6(2^{3-\alpha_4}) + 5^{2-\alpha_4}(2+\alpha_4) - 4 = 0$ we have

$$Q^*_4 = \begin{cases} 10a_{4,0} + 3a_{4,1} - 4a_{4,2} + 2a_{4,3} + 2a_{4,4}, & 1 < \alpha \leq \alpha_3 \\ 9a_{4,0} + 3a_{4,1} - 2a_{4,2} - 2a_{4,3} + 4a_{4,4}, & \alpha_3 \leq \alpha < 2 \end{cases}$$

$$Q^*_5 = \begin{cases} 8a_{5,0} - 3a_{5,1} + 2a_{5,2} + 2a_{5,5}, & 1 < \alpha \leq \alpha_4 \\ -10a_{5,0} - 3a_{5,1} + 4a_{5,2} - 4a_{5,3} + 2a_{5,4} + 2a_{5,5}, & \alpha_4 \leq \alpha \leq \alpha_1 \\ -10a_{5,0} - 3a_{5,1} + 4a_{5,2} - 2a_{5,4} + 4a_{5,5}, & \alpha_1 \leq \alpha < 2. \end{cases}$$

The values of α_3 and α_4 are approximately given by $\alpha_3 \simeq 1.6105$ and $\alpha_4 \simeq 1.4835$. For $j \geq 6$, Q_j^* becomes

$$Q_j^* = \begin{cases} -3a_{j,1} - 2a_{j,3} - 2a_{j,j-2} + 2a_{j,j-1} + 2a_{j,j}, & 1 < \alpha \leq \alpha_1 \\ -3a_{j,1} - 2a_{j,3} - 2a_{j,j-1} + 4a_{j,j}, & \alpha_1 \leq \alpha < 2. \end{cases}$$

We conclude that $||\mathbf{Q}^*||_\infty = Q_1^* = 10(\alpha - 2) + 3$ for $1 < \alpha \leq \alpha^*$ and $||\mathbf{Q}^*||_\infty = Q_4^* = 3^{3-\alpha} + 52^{3-\alpha} + 4^{2-\alpha}(-9\alpha + 3) + 6$ for $\alpha^* \leq \alpha < 2$, where α^* is such that $Q_1^* = Q_4^*$, that is, $\alpha^* \simeq 1.9118$. ■

Remark: From (18) of the previous proposition we can conclude that

$$||\mathbf{Q}^*||_\infty \leq ||\mathbf{M}^*||_\infty + ||\mathbf{N}^*||_\infty \leq 4 + 10 \max_{1 \leq j \leq N-1} |a_{j,0}|. \tag{20}$$

Since $||\mathbf{N}^*||_\infty \geq 10|a_{1,0}| = 10(2-\alpha)$, the inequality (20) leads to a larger upper bound than the one given by (19).

Additionally, if the diffusive coefficient of equation (1) is constant, such that, $d(x) = d$, then

$$||\mathbf{Q}||_\infty = \frac{||\mu^\alpha||_\infty}{2\Gamma(4-\alpha)} q_{\max}(\alpha).$$

The following theorem proves the numerical method is C-stable and from Theorem 3 we can conclude the method converges.

Theorem 5. *Let* $||d||_\infty = \max_{1 \leq j \leq N-1} d(x_j)$. *If* $\Delta t < \dfrac{2\Gamma(4-\alpha)\Delta x^\alpha}{||d||_\infty q_{\max}(\alpha)}$, *then the numerical method (16) is C-stable.*

Proof: Let U^n and $\tilde{U}^n$ be two solutions of the numerical method (16) and consider $e_n = \tilde{U}^n - U^n$. We have

$$e_{n+1}(I - \mathbf{Q}) = (I + \mathbf{Q})e_n,$$

that is,

$$e_{n+1} = e_n + \mathbf{Q}(e_{n+1} + e_n).$$

Therefore,

$$||e_{n+1}||_\infty \leq ||e_n||_\infty + ||\mathbf{Q}||_\infty \left(||e_{n+1}||_\infty + ||e_n||_\infty\right)$$

leading to

$$\left(1 - ||\mathbf{Q}||_\infty\right) ||e_{n+1}||_\infty \leq \left(1 + ||\mathbf{Q}||_\infty\right) ||e_n||_\infty.$$

Hence, by the previous proposition,

$$||e_{n+1}||_\infty \leq \frac{1+\Delta t C(\alpha)}{1-\Delta t C(\alpha)}||e_n||_\infty,$$

for $C(\alpha) = \dfrac{q_{\max}(\alpha)}{2\Gamma(4-\alpha)}\dfrac{||d||_\infty}{\Delta x^\alpha}$. We can therefore conclude the numerical method is C-stable. ■

Remark: If the physical boundary (13) is given, then $||\mathbf{Q}||_\infty = ||\mathbf{M}||_\infty$ and the condition of the previous theorem becomes

$$\Delta t < \frac{\Gamma(4-\alpha)\Delta x^\alpha}{2||d||_\infty}.$$

Many times the eigenvalue condition is used to prove the stability of a numerical scheme although it does not give reliable conditions. The eigenvalue condition is only a necessary condition for stability when we have an iterative matrix which is non-normal. In our case the iterative matrix is given by $(I-\mathbf{Q})^{-1}(I+\mathbf{Q})$.

5. Numerical results

We consider the same test problem presented in [14] for $\alpha = 1.8$ on a finite domain $0 < x < 1$, with the diffusion coefficient $d(x) = \Gamma(2.2)x^{2.8}/6$ and source function $p(x,t) = -(1+x)\mathrm{e}^{-t}x^3$. The initial condition is

$$u(x,0) = x^3, \quad \text{for} \quad 0 < x < 1$$

and the boundary conditions

$$u(0,t) = 0, \quad u(1,t) = \mathrm{e}^{-t} \quad \text{for} \quad t > 0.$$

The exact solution of the problem is of the form

$$u(x,t) = \mathrm{e}^{-t}x^3, \tag{21}$$

and is displayed in Figure 1.

In this section additionally to our numerical method we present results for the numerical method with the discrete approximation in space for the fractional derivative of order α defined from the shifted Grünwald-Letnikov

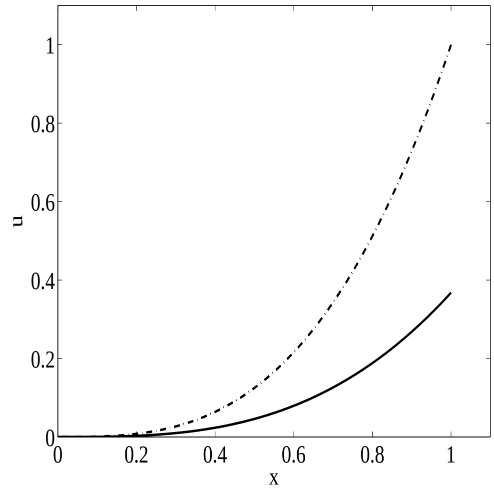

FIGURE 1. Exact solution (21) for $t = 0$ $(- \cdot -)$ and $t = 1$ $(-)$.

formula

$$\left(\frac{\partial^\alpha u}{\partial x^\alpha}\right)_j^n \simeq \frac{1}{\Delta x^\alpha} \sum_{k=0}^{N+j+1} (-1)^k \left(\begin{array}{c}\alpha\\ k\end{array}\right) U_{j+1-k}^n. \tag{22}$$

The time discretisation is still the Crank-Nicolson method, that is, for

$$\delta_\alpha^{gl} = \frac{1}{\Delta x^\alpha} \sum_{k=0}^{N+j+1} (-1)^k \left(\begin{array}{c}\alpha\\ k\end{array}\right) U_{j+1-k}^n,$$

we have the numerical method

$$\left(1 - \frac{\mu_j^\alpha}{2}\delta_\alpha^{gl}\right) U_j^{n+1} = \left(1 + \frac{\mu_j^\alpha}{2}\delta_\alpha^{gl}\right) U_j^n + p_j^{n+1/2}\Delta t. \tag{23}$$

The approximation (22), for $\alpha = 2$, is the second order central difference operator δ^2 and therefore the numerical method (22) is second order. Unfortunately, as reported in [14] and as can be seen in Table 1, this numerical method gives first order approximations when $1 < \alpha < 2$.

Consider the vectors $U_{app} = (U(x_0, t), \ldots, U(x_N, t))$, where U is the approximated solution and $u_{ex} = (u(x_0, t), \ldots, u(x_N, t))$, where u is the exact solution. The error is defined by

$$||u_{ex}(\Delta x) - U_{app}(\Delta x)||_\infty, \tag{24}$$

where $|| \cdot ||_\infty$ is the l_∞ norm.

The results in Table 1 for the numerical method (16) were obtained by considering the numerical boundary condition (14) since we did not consider a physical boundary of the form (13).

Δx	Grünwald Method (22)	Rate	Caputo Method (16)	Rate
1/10	0.1822×10^{-4}		0.1813×10^{-5}	
1/15	0.1168×10^{-4}	1.09	0.7983×10^{-6}	2.02
1/20	0.8648×10^{-5}	1.04	0.4523×10^{-6}	1.97
1/25	0.6849×10^{-5}	1.04	0.2888×10^{-6}	2.01

TABLE 1. Global l_∞ error (24) of time converged solution for four mesh resolutions at $t = 1$ for $\alpha = 1.8$ and its rate of convergence.

We observe the numerical method presented is second order accurate.

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